Equivariant Diffusion for Molecule Generation in 3D

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Abstract

This work introduces a diffusion model for molecule generation in 3D that is equivariant to Euclidean transformations. Our E(3) Equivariant Diffusion Model (EDM) learns to denoise a diffusion process with an equivariant network that jointly operates on both continuous (atom coordinates) and categorical features (atom types). In addition, we provide a probabilistic analysis which admits likelihood computation of molecules using our model. Experimentally, the proposed method significantly outperforms previous 3D molecular generative methods regarding the quality of generated samples and efficiency at training time.